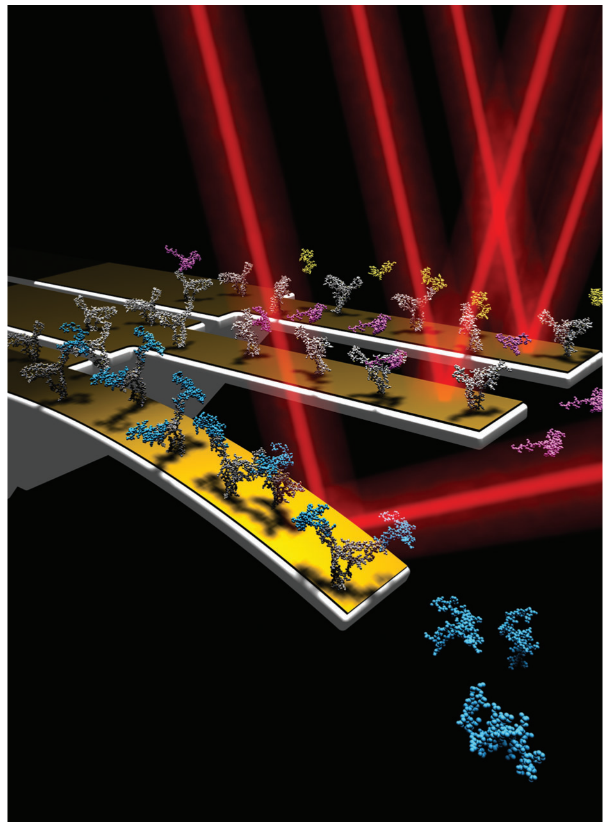
Investment Mode 2: NNI Grand Challenge Areas

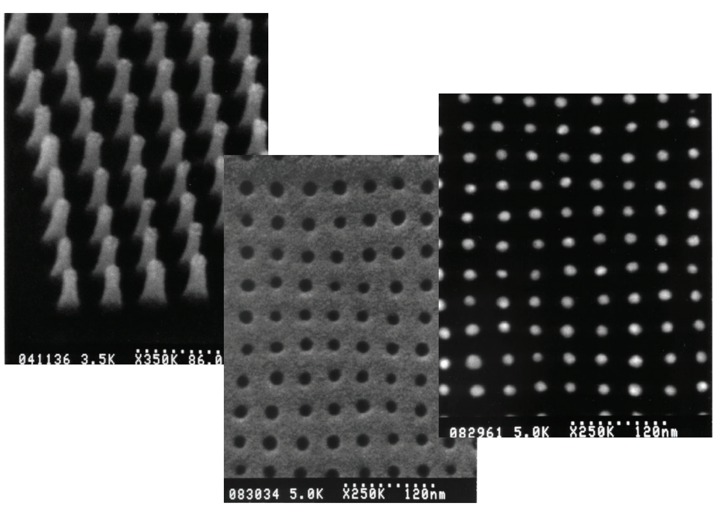
This section provides an overview of the nine grand challenge areas. Each overview covers the specific challenge area, a vision of how nanotechnology can drive progress in that area, the participating agencies, and an example demonstrating the progress that has been made to date.

The grand challenge areas are presented in the following order:

- Nanostructured Materials by Design
- Manufacturing at the Nanoscale
- Chemical-Biological-Radiological-Explosive Detection and Protection
- Nanoscale Instrumentation and Metrology
- Nano-Electronics, -Photonics, and -Magnetics
- Healthcare, Therapeutics, and Diagnostics
- Energy Conversion and Storage
- Microcraft and Robotics
- Nanoscale Processes for Environmental Improvement



(Above) Silicon cantilevers with chemically or biologically selective coatings for a biochemo-opto-mechanical chip. Adsorption of the target molecules on the coatings produces an expansion of the coating, resulting in deflection of the cantilever. Cantilever deflection can be sensed via light deflection as shown in the figure or by diffraction of light from interdigital fingers formed on the cantilever. This device provides the potential for rapid, sensitive, cost-effective detection of biomolecules and chemical species (courtesy A. Majumdar, University of California, Berkeley, and Lawrence Berkeley National Laboratory).



(Far left) Imprint mold with 10 nm diameter pillars. *(Left center)* 10 nm diameter holes imprinted in a polymer substrate. *(Near left)* 10 nm metal dots fabricated using a template such as in the center picture (courtesy S. Chou, Princeton University).

Grand Challenge Area Nanostructured Materials by Design

Challenge

Nanoscience involves structures with a limited number of atoms or molecules, larger numbers than traditionally handled by chemistry and smaller numbers than traditionally handled by materials science or solid-state physics. This departure from traditional material sizes can fundamentally change the way nanostructured materials behave, such that their properties frequently cannot be predicted from current models of materials behavior.

One reason for the difference in the properties of nanoscale materials compared to the analogous macroscale, or bulk, material is the large surface area per unit volume. Atoms at surfaces often behave differently from those located in the interior of a grain or particle. In addition, tiny variations in the structure and composition of nanostructured materials can have a dramatic effect on their properties. As a result, many important physical and chemical interactions, like catalysis, take place at surfaces or interfaces and, because of the high surface area and unique properties, are enhanced in nanostructured materials.

Other properties, such as magnetism and electrical and heat conductivity can change substantially as size is reduced to the nanoscale. The differences in these properties stem from surprising collective effects and so-called quantum-size effects that arise from the confinement of electrons in nanometer-sized structures.

Vision

When manufactured into usable products, nanostructured materials manifest the unique properties of their component parts. By gaining understanding and control at the nanoscale, materials scientists will be able to develop novel, high-performance, affordable, and environmentally benign materials. These novel materials could be custom designed for special purposes, having structural, optical, electronic, magnetic, and/or other special properties suited to their intended uses.

Modeling and simulation, aided by the expected continued advances in computational power, will play a major role in the realization of this vision. With the relatively small number of atoms contained in nanostructures, their properties can be predicted with increasingly accurate and fundamental models of atomic interactions. Therefore, theory and experimentation are expected to be highly interactive.

Agency Participation

(lead in bold)

DOD	Improved armor, high strength-to-weight materials, lower life-cycle costs
DOE	Modeling/simulation, energy storage/ transmission, friction, wear, corrosion
DOT	Improved materials and systems for transportation infrastructure
FDA	New or improved pharmaceuticals, cosmetics, biologicals, and medical device implant materials
IA	Materials-by-design for intelligence applications
NASA	High-performance, low-weight materials for space
NIST	Standard reference materials, materials property data, materials characterization methods
NSF	Novel structures, synthesis, and processing methods
USDA	Nanostructured materials from agricultural origins, nanocomposite polymers to enhance packaging functionality

Research Example: Molecular Perfection – The Fullerene Ideal (supported by DOD, NASA, and NSF)

Imagine a soccer ball shrunk to one billionth of its normal size. In 1985 researchers at Rice University created a geodesic-sphere-shaped molecule made of 60 carbon atoms (C60), dubbed the "buckyball." It was the first of a new class of molecularly perfect nanostructures now called fullerenes, named after the American architect Richard Buckminster Fuller.

The C60 molecule was soon followed by other fullerenes containing many more atoms of carbon and taking different shapes. One of the most interesting of these is the "buckytube," or carbon nanotube (CNT), an elongated nanoscale tube made entirely out of carbon. A computer model of a CNT is shown in Figure 7.

CNTs have unique properties, which, like those of diamond, arise from its perfect structure. Depending on the precise pattern of the carbon network, a CNT can act as either a highly conductive metal wire only one nanometer in diameter, or as a semiconductor. It has been used to build the first room-temperature transistor ever made from a single molecule, and is widely expected to be the key ingredient in nanoelectronics that will vastly extend the power and shrink the size of computers and other "smart" devices. Carbon nanotubes are also efficient electron emitters, which may lead to their application in affordable flat panel displays.

In addition to their remarkable electrical properties, carbon nanotubes are incredibly strong. Pulled end-to-end, a CNT has a tensile strength about 30 times greater than that of steel, while having only 1/6th its weight, making it the strongest fiber ever made. Researchers at the University of Texas at Dallas, with funding from the Defense Advanced Research Projects Agency in DOD, have woven fabric from fibers spun from a composite of polymers and CNTs. The new CNT-based fiber has a very high breaking strength and can be used to replace materials like Kevlar in bulletproof vests and other applications.

Finally, the thermal conductivity down the length of a single carbon nanotube has been measured to be 50% higher than diamond – previously the material with the highest known thermal conductivity – making it a superb material for piping heat from one place to another. Heat removal is a key issue, for example, in computers and other high-density electronic devices.

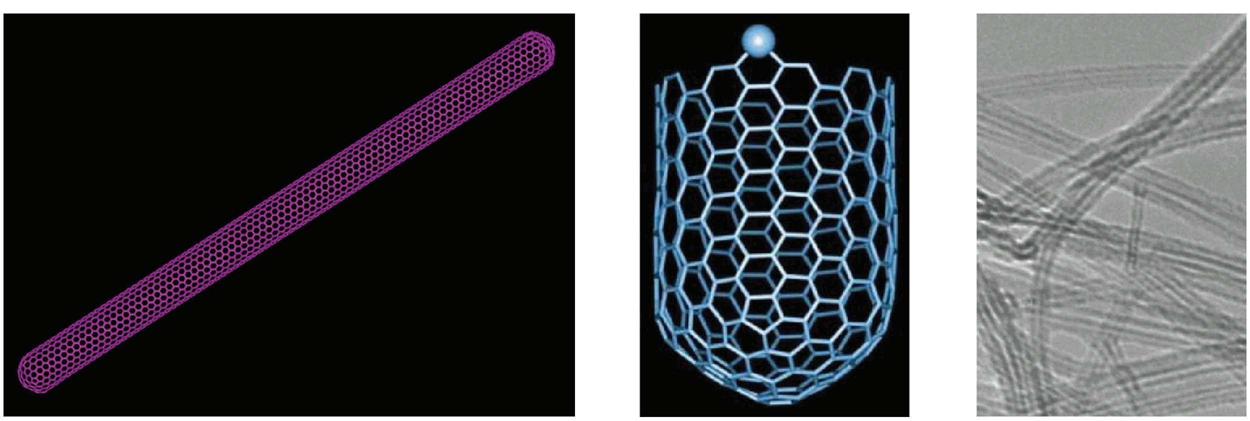


Figure 7. Single-walled carbon nanotubes. (Left) Computer drawing (courtesy Richard Smalley, Rice University). (Center) Enlarged view of computer drawing; (Right) High-resolution electron micrograph of nanotubes (courtesy NASA).

Grand Challenge Area

Manufacturing at the Nanoscale: New Methods for Traditional and Emerging Technologies

Challenge

Because nanostructures have little mass and are dominated by surface-area effects and size effects, the processes and equipment for nanotechnology-based manufacturing are expected to differ significantly from those currently used. Nanofabrication thus requires the invention of new instruments, measurement tools, models, methods, and standards to characterize nanoscale materials and processes. Only through such developments can the manufacture of commercial volumes of products—with a high degree of repeatability—become economically viable. Manufacturing at the nanoscale is a central challenge for the NNI because it is a prerequisite for realizing the benefits of nanotechnology. A concomitant challenge is the creation of high quality, diverse nanoscale building blocks that enable their assembly into large systems.

Vision

Manufacturing at any scale is a complex endeavor involving the use of many types of equipment and processes to transform raw materials into tangible products with desired properties or performance characteristics, generally in large quantities. Atoms and molecules are the raw materials for nanotechnology-based manufacturing. And only those raw materials that will become part of the final product will be selected for the nanofabrication process.

This bottom-up approach differs greatly from that of current manufacturing processes that involve assembling large quantities of materials, from which product parts are cast, machined or otherwise derived and waste products are left for disposal.

Nanostructured materials, devices, and systems will be manufactured with precise control over the location of individual atoms and molecules. The resulting nanoscale components will be hierarchically integrated and incorporated into macroscale devices and systems. Innovative ideas will be required to allow for nanoscale positioning; addition and removal of material; directed self-assembly; and biomimetic (i.e., life-imitating) fabrication paradigms.

Since an entirely new approach to manufacturing is required, there is a need to concurrently develop new tools and facilities to support this effort.

Agency Participation

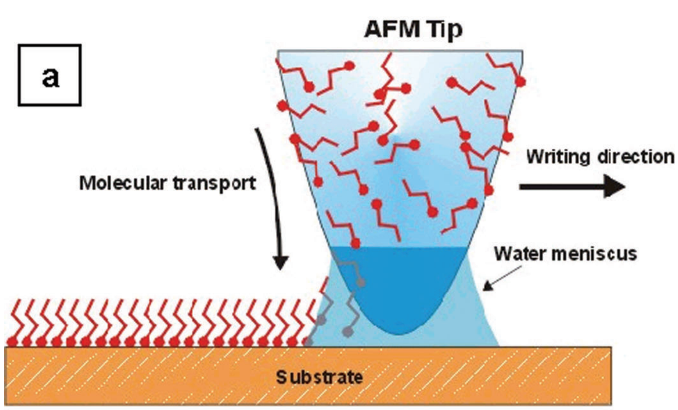
(leads in bold)

DOE	Novel synthesis and processing approaches
EPA	"Green manufacturing" with minimal waste streams
IA	Prototype functional nanodevices
NIST	Measurement technology and standards for process characterization and quality control
NSF	Research for manufacturing processes, new theoretical models, and simulations
USDA	Biological manufacturing

In addition to the above agencies, which have specific efforts in manufacturing at the nanoscale, each NNI agency is committed to this grand challenge area and will incorporate it into their plans as appropriate to their respective mission-specific programs.

Research Example: Dip-pen Nanolithography—A new approach to nanoscale fabrication (supported by NSF and DOD)

The ability to make nanoscale patterns on surfaces is a critical process in, for example, the manufacture of electronic circuits, the performance of high-throughput biomedical research, and the design of advanced sensors. However, the cost of extending currently used methods to smaller and smaller scales is substantial. Researchers at Northwestern University have developed a new approach called "Dip-Pen Nanolithography" (DPN) that utilizes an atomic force microscope tip as an "ink pen" (Figure 8). DPN is a direct, single-step process that does not require the use of patterned masks or light-sensitive films, or other steps to form patterns on a substrate. Additionally, it may be performed under ambient conditions. DPN provides a reliable approach to writing nanoscale lines of a variety of molecules onto various solid surfaces. Repetitive patterns of nanoscale lines may be created in parallel using an array of writing tips. The inventors of the DPN technology have formed a start-up company that plans to develop products and services for the fabrication of patterned nanostructures.



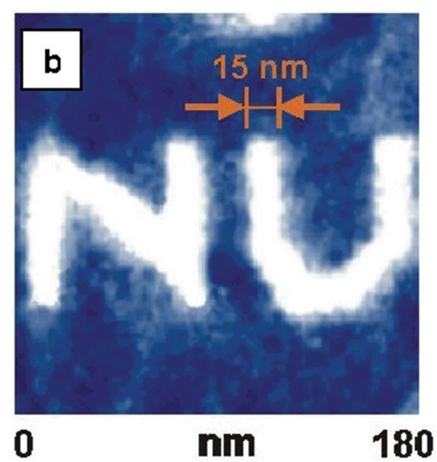


Figure 8. (a) Cartoon showing how dip-pen nanolithography "writes" molecules onto a substrate. A major advantage of this process is that it creates a nanostructure pattern on a surface in one step. Conventional processes to create such a patterned nanostructure require up to five complex steps and very sophisticated fabrication tools. (b) Linear force microscope image of an acid "ink" patterned on a gold substrate. The patterned feature size is 15 nm and spatial resolution is ~5 nm (courtesy C. Mirkin, Northwestern University).

Grand Challenge Area

Chemical-Biological-Radiological-Explosive (CBRE) Detection and Protection: The Application of Nanotechnology to Homeland Defense

Challenge

Conventional explosives have been the weapon of choice for terrorists, and their use remains a serious threat to the Nation's security. At the same time, the recognition that small amounts of chemical, biological, or radiological agents can exact a much greater human toll than an equivalent amount of explosives has prompted the need for additional precautions and mitigation methods. New technologies that reliably and rapidly detect trace amounts of chemical, biological, radiological, or explosive materials are critical to the national defense, as are new technologies to protect people from the devastating effects of these substances.

Vision

Nanotechnology offers the potential for unprecedented improvements in the sensitivity, selectivity, response time, and affordability of detection technologies. Nanoscience and nanostructures also offer the opportunity for revolutionary advances in adsorbent materials (personal and collective protection), separation technologies (protective clothing and filters), decontamination and neutralization of agents, and prophylactic measures.

One key objective for this grand challenge area is the development of miniaturized intelligent sensors. Such devices would have the potential to sense the presence of specific molecules with accuracy and sensitivity well beyond what is commercially available today. Building such devices will require a much better understanding of nanoscale forces and interactions.

Another key objective is to develop novel protection, neutralization, and prevention technologies. Protective masks and clothing depend on high surface area materials. Nanostructures inherently have large surface-to-volume ratios and also tend to have highly reactive surfaces that may neutralize the toxic material rather than simply hold it. Nanostructures also can be tailored to selectively disrupt the biological activity of pathogens.

Agency Participation

(lead in bold)

DOD	Detection of and protection against CBRE agents
DOE	System integration, lab-on-a-chip, CBRE detection
DHS	Detection of and protection against CBRE agents
DOT	Advanced transportation security systems
EPA	Reduction and remediation of hazardous material
FDA	Processes to ensure safety and security of the food chain
IA	Detection of CBRE agents
NASA	System integration, miniaturization, robotic systems
NIH	Detection of and treatment for chemical, biological, and radiological exposure
NIST	Chemical microsensors, single-molecule measurement
NSF	Sensors and basic principles for detection of and protection against CBRE agents
USDA	Processes and detection techniques to secure agricultural production and food resources

Note: The NNI works closely in this area with the interagency Technical Support Working Group (TSWG), which coordinates efforts in CBRE detection as part of its mission to facilitate development of technologies to combat terrorism.

Research Example: Cantilever Array for Chemical and Biological Threat Analysis (supported by DOE)

Experience with the micro-cantilevered probes used in atomic force microscopes has stimulated the development by various researchers of nanoscale cantilever-based physical, chemical, and biological sensors. Extending the fabrication techniques for microelectromechanical systems (MEMS) to produce devices with nanoscale components not only allows for even smaller and lighter detectors, but also enhances sensitivity. Demonstrated applications include detection of chemical warfare agents, alpha particles, biomolecules, TNT, and plastic explosives. It is possible to arrange arrays of micro- and nano-cantilevers on a single chip to allow detection of multiple targets or to extend the dynamic range (i.e., range of concentrations that can be detected).

One cantilever-based approach detects adsorbed molecules by measuring the change in resonance frequency of individual cantilevers. In general, the smaller the cantilever, the higher its resonance frequency will be and the greater its sensitivity. To date, frequencies from one megahertz to over one gigahertz have been achieved by pushing the cantilever dimensions into the nanometer scale. Whereas cantilever geometry determines sensitivity, selectivity is controlled by coating the cantilever surface with compounds that bind only to the molecule of interest. Researchers at Oak Ridge National Laboratory have developed a cantilever sensor (Figure 9) that uses this approach to detect the presence of nanoscale quantities of material. By having a range of cantilever shapes, and hence frequencies, the sensor array is able to detect a wide range of molecular concentrations. In addition, individual cantilevers may be treated with different coatings to allow detection of multiple target compounds. The Oak Ridge team has demonstrated the ability to detect certain agents down to the single molecule level.

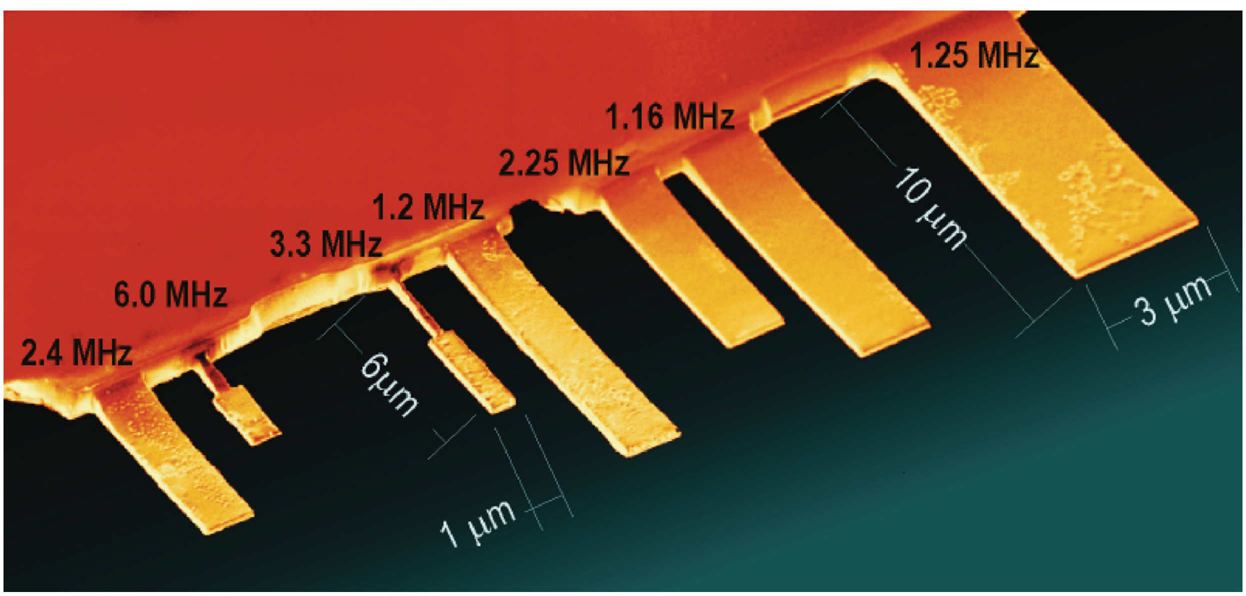


Figure 9. Scanning electron micrograph of an array of silicon cantilevers, milled to various dimensions with a range of resonance frequencies. Detection of adsorbed molecules is achieved by measuring frequency shifts. The cantilevers shown here are coated with gold, which allows detection of as little as a few femtograms (10^{-15} g) of an acidic test compound (courtesy P. Datskos, Oak Ridge National Laboratory).

Grand Challenge Area

Nanoscale Instrumentation and Metrology: A New Age of Measurement Standards and Tools

Challenge

Nanotechnology-based industry requires the development of highly capable, low-cost, reliable instrumentation and internationally accepted standards for the measurement of nanoscale phenomena and for the characterization and manipulation of nanostructures. Improvement in measurement and manipulation capabilities is critical to the progress of nanotechnology.

Vision

Improved measurement methods to better characterize nanoscale processes and structures are needed. Additionally, present nanoscale measurements have little metrological underpinning and few standards to ensure their reliability and repeatability. Standard reference materials need to be developed and calibrated to establish the accuracy and reproducibility of a given nanoscale measurement tool. Standardized instruments with nanoscale resolution will accelerate scientific discovery and provide quality control in the fabrication and assembly of manufactured nanostructures. These research tools also will be adapted into miniaturized sensor and actuator technologies.

The complexity and breadth of nanotechnology provides a wealth of opportunities for innovation in instrumentation and metrology. Analytical instrumentation with increased resolution and sensitivity is needed to characterize the chemical composition and structure of materials at the nanoscale. Quantitative models for interpretation of scanned probe images are lacking. New analytical approaches are needed to characterize soft materials—materials otherwise deformed by the proximity of tips used in scanning probe microscopes. Progress in understanding biological systems is severely hampered by inadequate capability for probing cellular and subcellular nanoscale phenomena. Instrumentation for precise nanometer-position control across samples of centimeter dimensions will be required to realize commercial nanoscale device fabrication.

The creation of atomically controlled and measured structures may lead to the establishment of new fundamental standards. For example, quantized electron devices may provide improved electrical current standards.

Agency Participation
(leads in bold)

DOE	Centers to exploit unique national laboratory measurement capabilities
NIH	*In situ* diagnostics and therapeutics, medical imaging
NIST	Nanoscale measurement science, instrument calibration, standard reference materials, and nanoscale physical and chemical properties standard reference data
NSF	Broad based science as a source of new instrumentation concepts

In addition, DOD, DOE, EPA, IA, FDA, NASA, and DHS are developing measurement instrumentation with improved signal-to-noise for more sensitive detectors for each agency's mission-related needs.

Research Example: State-of-the-Art Nanoscale Measurement and Manipulation (supported by NIST)

Propelled by the constant need for increased speed and density and reduced cost, electronic and magnetic devices continue to get smaller. Integrated circuits in present day electronic devices have dimensions of less than 100 nanometers. Measurement of such nanostructures demands novel fabrication and characterization systems, such as illustrated in Figure 10. The facility shown here enables the atom-by-atom assembly of complex nanostructures under completely autonomous computer control. The facility is designed with the goal of atomic-resolution imaging and the ability to probe electronic properties of nanostructures with high-electron energy resolution. Cryogenic temperatures are required to achieve electron energy measurements sufficient to resolve the variation of quantum energy states in nanostructures. *In situ* fabrication and transfer of samples is essential to the study of well-designed and characterized nanostructures.

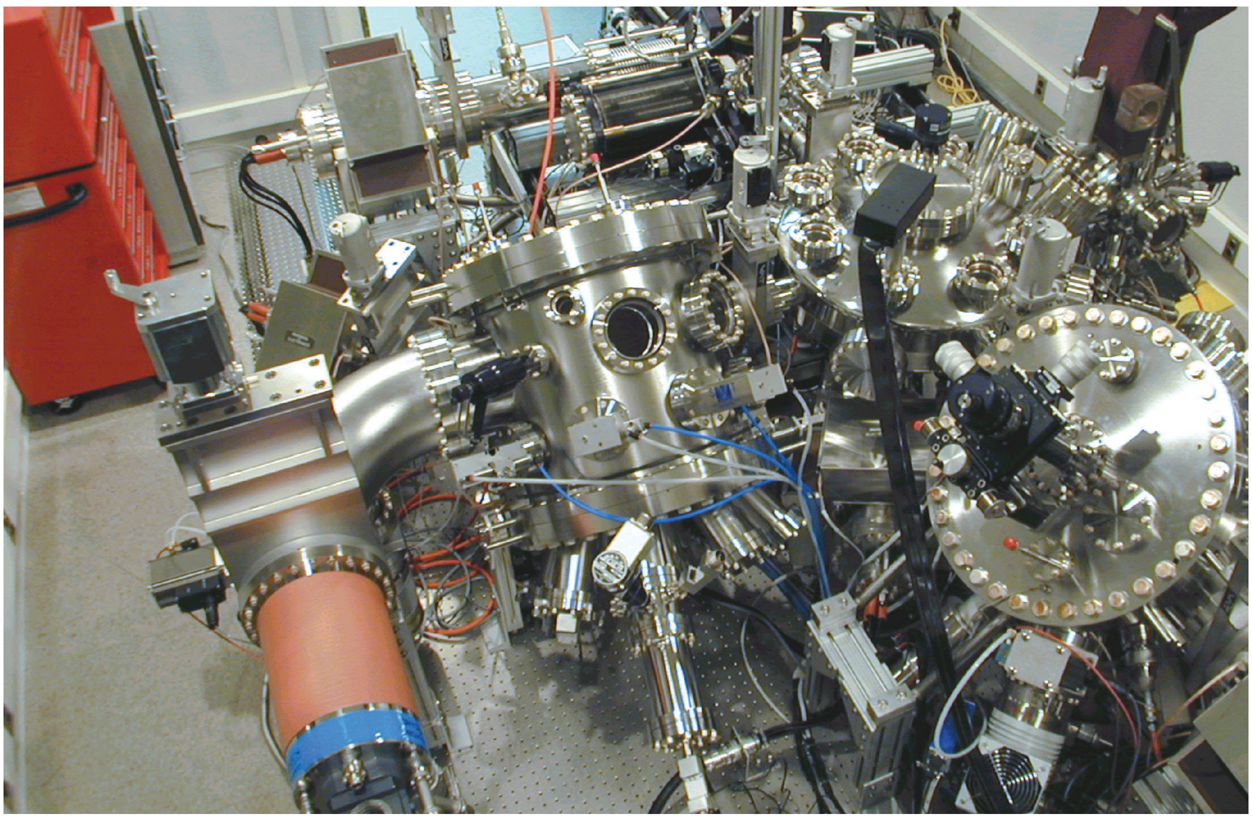


Figure 10. The NIST Nanoscale Physics Facility is a unique state-of-the-art instrument for the fabrication, characterization, and manipulation of novel nanostructures, with the following specific capabilities:

- Scanning tunneling microscope operating at ultra-high vacuum and controlled temperatures from about -270˚C to -150˚C
- Superconducting magnet system with 1.5 Tesla vector magnetic fields at the microscope position and 10 Tesla vertical magnetic fields at the microscope position
- Molecular beam epitaxy system to deposit semiconductors and metals with *in-situ* transfer of samples to the scanning tunneling microscope system
- Tip preparation system to image the atomic structure of tips with *in-situ* transfer of tips to the scanning tunneling microscope system
- Acoustically and electrically shielded measurement environment with extraordinarily high attenuation of external environmental disturbances

Courtesy J.A. Stroscio and R.J. Celotta, NIST Physics Laboratory

Grand Challenge Area

Nano-Electronics, -Photonics, and -Magnetics: The Next Generation of Information Technology Devices

Challenge

Further miniaturization of microelectronics – with more functionality and at lower cost – will require new approaches to fabrication and processing, and new methods for acquiring, storing, processing, transmitting, and displaying data.

Vision

Nano-electronic systems offer the potential to sustain the revolution in information technology devices provided by silicon-based micro electronics over the last 30 years. Nano-based systems will improve computer speed, expand mass storage, and reduce power consumption. Communication paradigms will change by increasing bandwidth for data transmission, and by developing flexible, flat displays that are many times brighter than conventional displays.

The physics of today's transistor devices does not scale to the length of a few nanometers. The properties of nanostructures need to be measured and incorporated into new device concepts, and the devices placed into new system architectures.

Without breakthroughs, the continued miniaturization of information technology devices may stall, due in part to economically unacceptable increases in manufacturing costs. The cost of a single fabrication plant for 65 nanometer electronic devices is now estimated at approximately $4 billion. Therefore, it is necessary to identify novel synthesis, processing, and manufacturing technologies such as (a) printing and stamping approaches to pattern transfer; (b) processing of devices in parallel via arrays of microelectromechanical systems (MEMS) technologies; (c) innovations in surface processing, controlled nucleation, directional growth, and directional etching innovations; and (d) batch formation of precursor nanostructures followed by directed self-assembly.

Agency Participation

(leads in bold)

DOD	Devices for communication, command, control, surveillance, and reconnaissance
DOE	MEMS, laboratory-on-a-chip
IA	Molecular electronics and advanced communication systems
NASA	Highly effective, miniaturized, low-power devices for spacecraft
NIST	Standards for measurement, manufacturing quality control
NSF	Novel phenomena, devices, and architectures

Research Example: Molecular Electronics—Nanowire interconnects (supported by DOD and NSF)

Researchers have been working on molecular-scale electronics devices for years. Advances in this field may extend the famous "Moore's Law" for an additional 10 to 20 years, or well beyond the fundamental limits of purely silicon-based technology. Moore's law describes the exponential growth of computational power over time, and has become a standard guide by which computational manufacturers judge their technological advancements.

One concept for molecular electronics comes from the work of researchers at Hewlett-Packard (HP), the California Institute of Technology and the University of California at Los Angeles (UCLA). They have placed a particular molecule, a rotaxane, into one of two electrically distinct states that correlate to a "0" or a "1." This approach preserves the digital nature of electronics and permits the current approach for memory and logic to be carried forward. The most complex elements of logic and memory can be extracted from such a molecular electronic "bit," which is formed by a few rotaxane molecules that are "sandwiched" between two crossed wires. Thus, the rotaxane or a similar molecule can be arranged to represent digital logic and memory. An array of such bits (similar to an expanded tic-tac-toe board) allows for error-free computation even in the presence of defective components, a critical characteristic for many nanotechnologies.

An early application of this technology is as highly efficient, random access memory. Today, random access memories are patterned at a density of about 3×10^8 bits/cm^2. Using rotaxane switches, the HP, Caltech, and UCLA research team has demonstrated working memory and logic prototypes that are up to 100 times more dense than conventional devices (see Figure 11). Although certain challenges, such as interconnection, must yet be met in order to demonstrate working circuitry at these densities, this molecular electronics technology is already exceeding traditional approaches by orders of magnitude in laboratory demonstrations.

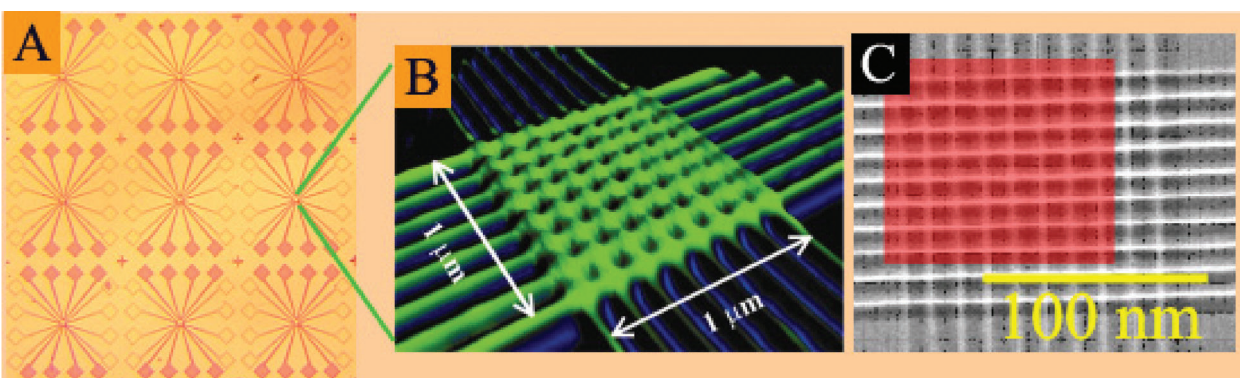


Figure 11. (A) Optical micrograph of an array of 64-bit molecular electronic circuits. (B) Atomic force micrograph revealing the detailed structure of one of the 64-bit circuits, patterned at a density of 7×10^9 bits/cm^2. This circuit has been utilized for simultaneous logic and memory operations. (C) The smallest circuit currently known (5×10^{11} bits/cm^2). As in (B), a bit is formed at each intersection of the lines. The highlighted 64 bits of this ultra-dense circuit fits inside a single bit of the circuit shown in (B) (courtesy J. Heath, Caltech).

Grand Challenge Area

Healthcare, Therapeutics, and Diagnostics: Using Nanotechnology for Better Disease Detection and Treatment

Challenge

Three critical areas within healthcare, therapeutics, and diagnostics lend themselves to nanoscale science and technology solutions. The first is improved implants developed by using biocompatible materials, tissue engineering, and regenerative medicine. The second is delivery of drugs, gene therapies, and other therapeutics. The third is earlier detection of disease, which could greatly enhance the success rate of existing treatment strategies and significantly advance our ability to employ prevention strategies.

Vision

Biological phenomena are largely governed by nanoscale structures. For example, the mechanisms of protein synthesis, replication, signal transduction, and infection occur at the nanoscale. Therefore, advances in a wide range of nanoscale science and technology will be relevant to biological research, and vice versa. Special opportunities exist for collaboration among life scientists and physical scientists. Collaborative programs leverage the knowledge base from each discipline, affording the best opportunities to shift life science paradigms from "hypothesis-driven" to mechanistic understanding.

As we achieve a better understanding of the design of biomolecular systems and learn how to build and control materials at this size scale, technologies for intervening in biological processes will emerge. These technologies offer promising routes to earlier detection of disease, more effective diagnostics and therapeutics, novel biocompatible materials, targeted gene and drug delivery systems, novel vision and hearing aids, and "smart" medical devices for treatment modes that minimize collateral damage.

Agency Participation

(lead in bold)

DOD	Casualty care, monitoring war fighter physiology, improving human capability to respond to threats
DOE	Radiation effects, sensors, hard/soft matter interfaces
FDA	Safety, efficacy, and quality assurance of drugs, medical devices, and biological products
NASA	Remote and autonomous medical care in space environment
NIH	Therapeutics, diagnostics, and regenerative medicine
NIST	Standards for bioscience and bioengineering
NSF	Nano-bioscience, nano-bioengineering
USDA	Food safety, animal health, plant disease prevention and treatment

Research Example: Peptide Nanotubes as Antibacterial Drugs (supported by NIH)

Bacterial resistance to antibiotics is a growing problem worldwide that is compromising the medical community's ability to treat many infectious diseases. Most antibiotics used today target invading bacteria by latching onto specific molecules in the bacteria's outer membrane. If the bacteria can modify those molecules even slightly, they become resistant to the antibiotic and can go on to infect their host.

Researchers at the Scripps Research Institute in San Diego have developed peptide nanotubes, shown schematically in Figure 12, that kill bacteria by punching holes in the bacteria's membrane. Each tube is formed from strings of amino acid subunits called peptides that, because of their structure, assemble into tiny rings. These rings stack on top of each other to form tubes on the order of barely one nanometer in diameter. By controlling the type of peptides used to build the rings, scientists are able to design nanotubes that selectively perforate bacterial membranes without harming the cells of the host.

In theory, these nano-bio agents should be far less prone than existing antibiotics to the development of bacterial resistance. The invading bacterium would have to substantially alter its membrane, not just alter a particular molecule, to become resistant to the nanotubes. Even if bacteria succeeded in altering their membranes, scientists could counter by modifying the structure of the nanotubes. Moreover, peptide nanotubes are resistant to proteases (protein-digesting enzymes found in the body) and therefore bypass a common problem in designing antibiotic agents.

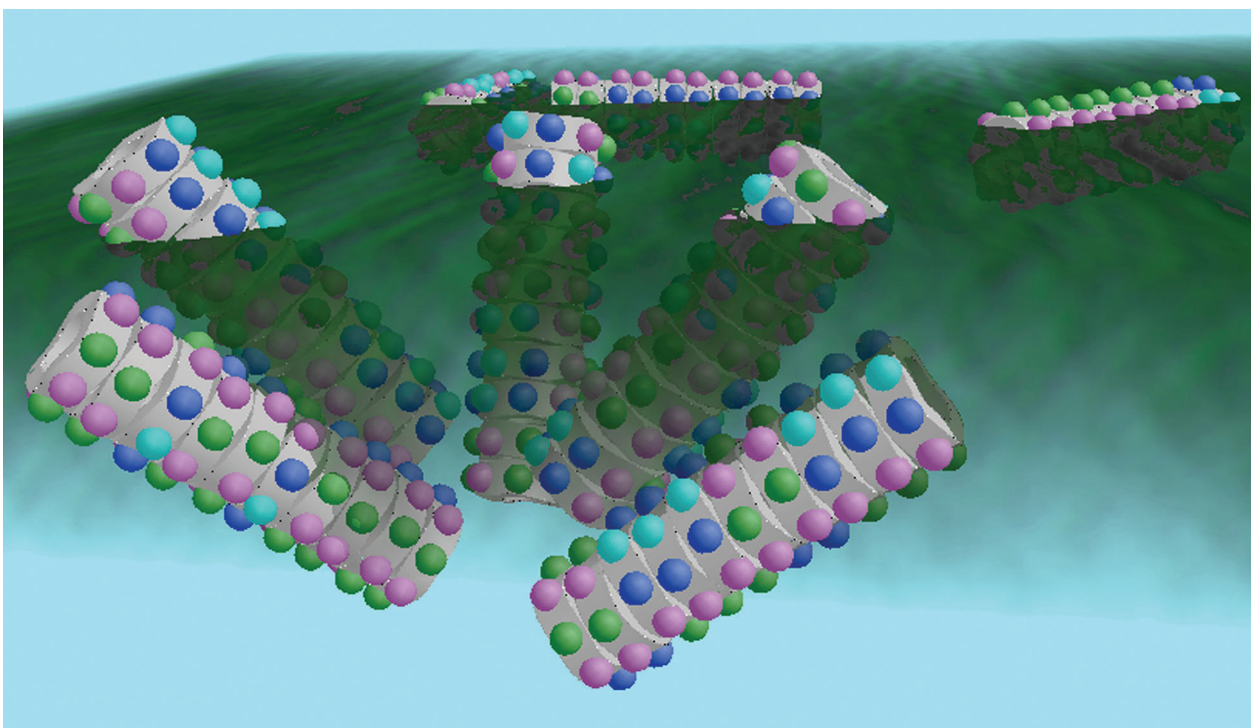


Figure 12. Schematic of designed peptide nanotubes that have penetrated a bacterial cell wall, effectively killing the bacterium. The nanotubes are formed from stacks of rings, which in turn are made up of various peptides (indicated by colored dots) (courtesy A. Olson and M.R. Ghadiri, Scripps Research Institute).

Grand Challenge Area

Energy Conversion and Storage: New Materials and Processes for Energy Needs

Challenge

Inexpensive energy underlies economic prosperity. A nation's ability to develop new energy sources within its own borders can reduce dependency on international energy supplies and finite oil reserves. Novel abilities and improved efficiencies in converting, storing, transmitting, and conserving energy are also critical to the challenge of providing clean, abundant, and secure energy for domestic needs.

Vision

Nanotechnology promises significant improvements in solar energy conversion and storage, thermoelectric converters, high-performance batteries and fuel cells, and efficient electrical power transmission lines. For example, nanoscale control of materials structure and composition has shown promise for novel approaches to photovoltaic systems. A deeper understanding of the physics of phonon and electron transport in nanostructured materials may facilitate production of practical all-solid-state and environmentally clean thermoelectric energy conversion devices. Currently, hard and soft magnets are widely used in electric power production and utilization. Improved nanostructured magnets may yield substantial energy savings by reducing losses incurred in the generation and use of electricity.

Nanostructures may also enhance the controlled release of chemical energy toward specific goals such as more efficient combustion, greater thrust in rocket propulsion, thermobaric destruction of chemical or biological agents, and tailored electromagnetic emission from propulsion systems (lower intensity signatures or better decoys to foil missile seekers). Nanoscale control of the shapes, chemistry, and phases of catalyst particles and supports clearly will impact energy conversion, chemical processing, and related fields.

Opportunities also exist for increasing thermal transport rates in fluids by utilizing nanocrystalline particulate suspensions. These "doped" nanofluids have recently been shown to exhibit substantially increased thermal conductivities and heat transfer rates compared to their "undoped" counterparts.

Agency Participation

(lead in bold)

DOD	Energetic materials for propulsion, decoys, explosives
DOE	All aspects of energy research, including catalysis, fuel cells, hydrogen
IA	Nano-enabled advanced power systems
NASA	Energy conversion and storage for space systems
NSF	Materials science and engineering
NIST	Manufacturing processes and equipment
USDA	Biomass conversion to energy and chemicals, hydrogen production, distributed power production

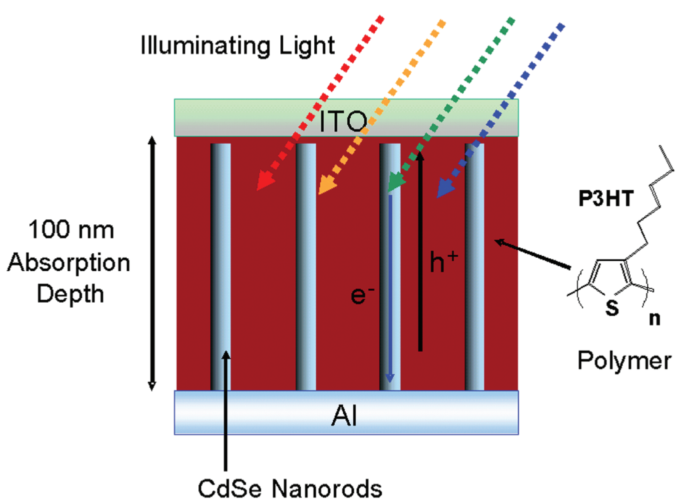
Research Example: Polymeric Nanostructures for Conversion of Solar Energy (supported by DOE)

Nanotechnology may provide a path to a new generation of solar cells. Presently, low-cost solar cells with power efficiencies of around 12% are readily available, while high-end solar cells with efficiencies of 34% can be made for satellites, but are prohibitively expensive for large-scale terrestrial applications. Researchers at the University of California at Berkeley and Lawrence Berkeley National Laboratory have reported a new type of “paint-on” solar cell that has promise for relatively low fabrication cost and the potential to achieve efficiencies comparable to those of high-end cells.

At the heart of all solar cells are two separate material layers, one with a reservoir of electrons that functions as the “negative pole,” and one having vacancies for electrons called electron holes that functions as the “positive pole” of the cell. Absorption of light from the sun or other light source by the cell provides energy to drive the electrons from the negative to the positive pole, creating a voltage difference between the two and thus enabling the cell to serve as a source of electrical energy.

The new devices are based on a combination of a semiconductor polymer (an organic material) and cadmium selenide nanorods (an inorganic material) (Figure 13). In this cell, each microscopic step in the performance of the solar cell is independently optimized. Absorption of light can occur in either the nanorods or the polymer, and charge separation takes place at the interface between them, followed by charge transport to the harvesting electrodes—indium tin oxide (ITO) and aluminum (Al).

Solar cells made with these devices have the potential to provide low-cost, ultra-lightweight, and flexible cells with a wide range of applications. Due to the nanoscale dimensions of the nanorods, quantum-size effects influence their optical properties. By tailoring the size of the rods, they can be made to absorb light within a specific narrow band of colors. By stacking several cells with different sized rods, a broad range of wavelengths across the solar spectrum can be collected and converted to energy. Moreover, the nanoscale volume of the rods leads to a significant reduction in the amount of semiconductor material needed compared to a conventional cell.



Transmission electron microscope image of a 7 nm by 30 nm CdSe manorod

Figure 13. Schematic design of the nanorod-polymer solar cell illustrating how light energy activates the polymer (P3HT) and cadmium selenide (CdSe) components of the cell to drive electrons (e-) and holes (h+) to opposing aluminum (Al) and indium-tin oxide (ITO) electrodes (courtesy P. Alivisatos, University of California, Berkeley, and Lawrence Berkeley National Laboratory).

Grand Challenge Area
Microcraft and Robotics

Challenge

Integrating the miniaturization of machinery and computers can provide platforms to operate in hazardous or confined environments without human presence and can augment productivity by automating more routine operations. For instance, reduced payload weight and energy usage are critical factors that impact our ability to reach ever more remote and hostile environments on Earth and in space. Miniaturized, intelligent machinery also will enable the development of other highly desirable systems such as unmanned military combat platforms that reduce risks to personnel and *in vivo* systems that improve the detection and treatment of disease.

Vision

Nanotechnology will provide the ability to design very small-scale microcraft, vehicles and robots. Microelectromechanical systems (MEMS) are already providing some system miniaturization down to the microscale. Building on the fabrication processes and devices of MEMS technologies, nanoelectromechanical systems (NEMS) will open qualitatively new functional approaches and applications.

Nanosystems based on biological principles and building blocks are a key area for future research. For instance, long duration missions or missions in hazardous environments may benefit greatly from adopting strategies and architectures from the biological world. Utilization of *in situ* resources to create complex structures and craft that can adapt and react to changing environmental or mission needs are examples of the kinds of advances enabled through the application of nanotechnology and the principles of molecular biology. If the application is *in vivo,* then the use of molecular motors fueled by the body's metabolites might even provide a "self-powered" system.

Sensing, processing, and managing information is critical to the control of any microcraft or robot. A compelling need exists for miniaturized electronics with increased capability that can be embedded in system controls. The development of ultra-lightweight and ultra-strong materials that can survive extreme environments will be key to expanding our reach into applications such as space exploration.

Agency Participation

(lead in bold)

DOD	Surveillance, unmanned combat platforms, improving human capability to respond to threats
FDA	Safety, efficacy, and quality assurance of medical products
IA	Novel robotic systems
NASA	Intelligent spacecraft, smart materials/ devices, autonomous healthcare systems
NIH	Telemedicine diagnostics/surgery; *in vivo* systems for diagnosis/therapeutics
NSF	Fundamental research on new principles and architectures for devices and systems
NIST	Intelligent systems research

Research Example: Molecular Motors—A New Nanoscale Biomimetic Paradigm for Energy Conversion (supported by NSF)

A biological cell has micrometer dimensions with the molecular machinery inside that cell having nanometer dimensions. Many cell functions require the action of "biological motors" that convert chemical energy to mechanical energy. For example, biological motors allow muscle fibers, flagella, and cilia to perform their functions.

One of the goals of researchers in this field is to develop an understanding of the mechanisms and processes of biological molecular motors and to incorporate similar approaches in nanoscale manmade devices. Researchers at Boston College have made steps toward this goal by designing and demonstrating a simple molecular motor that exhibits unidirectional rotary motion. The molecular motor consists of 78 atoms and consists of a rotating paddle-like structure attached to a base. Normally, thermally stimulated motion would cause this wheel-like molecule to rotate randomly in either direction. However, by tailoring the paddle wheel's molecular structure so that it is no longer entirely symmetrical, it can be induced to preferentially rotate in one direction. The impetus for rotation comes from chemical interaction between the paddle wheel part of the molecule and a common chloride compound, carbonyl dichloride. This particular molecular motor is not yet capable of continuous rotation—it rotates just 120 degrees—however, it represents a step toward being able to design nanoscale motors with controlled motion.

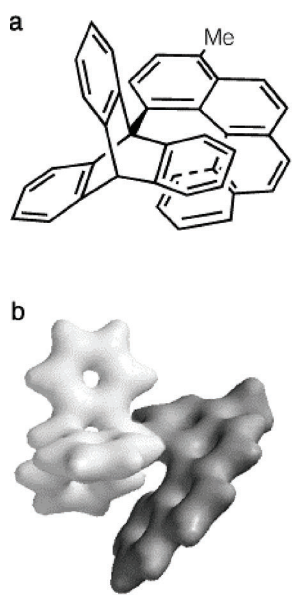


Figure 14. Diagram of a molecule designed to perform unidirectional rotary motion. The chemical structure is shown in (a). The molecule consists of two parts—a structure with three ringshaped paddles and a flat base—connected by a single bond about which rotation can occur. Figure 14(b) shows a calculated electron density surface map of the molecule as seen from a side view of the paddle wheel, which is shown in lighter gray. Upon interaction with carbonyl dichloride, the paddle wheel rotates 120 degrees in a clockwise direction (courtesy T.R. Kelly, Boston College).

Grand Challenge Area

Nanoscale Processes for Environmental Improvement

Challenge

Pollution has long been recognized as a serious threat to both the local and global environments and to our quality of life. The development of new technologies that enable industrial economies without harming human health and the environment is of critical importance in the 21st century. Development of innovative technologies for manufacturing, transportation, and other activities that reduce or eliminate the production of harmful by-products, or for treatment and remediation of existing toxic substances in the environment, presents major challenges for our society.

Vision

Nanoscale science and engineering can significantly improve our understanding of molecular processes that take place in the environment and help reduce pollution by leading to the development of new "green" technologies that minimize the use, production, and transportation of waste products, particularly toxic substances. Environmental remediation will be improved by the removal of contaminants from air and water supplies to levels currently unattainable, and by the continuous and real-time measurement of pollutants. In addition, increasing knowledge of the environmental, social, and human health implications of nanotechnology is crucial.

In order to understand the consequences of contaminants moving through the environment, interdisciplinary research is needed on molecular and nanoscale processes that take place at one or more of the interfaces or within nanoscale structures in natural systems. Such research includes studies of inorganic/inorganic, inorganic/organic, and organic/organic interfaces, with a focus on the specific processes dominated by small length scales. Separation science—exploiting the evolving capability to tailor nanostructured membranes—offers new opportunities to selectively extract contaminants from air, water, and soil.

Novel interdisciplinary research that adapts newly developed experimental, theoretical, and computational methods for characterizing nanostructures is needed. The community of scientists and engineers studying the fundamental properties of nanostructures must be connected with the community attempting to understand complex processes in the environment in order to hasten the integrated understanding of the environmental implications of nanoscale phenomena.

Agency Participation

(leads in bold)

DOE	Extraction of radionucleotides from otherwise benign materials
EPA	Detection, remediation, and prevention of environmental pollution
FDA	Ensuring safety and security of the food chain
NSF	Nanoscale processes in nature, "green" manufacturing
USDA	Agriculture technologies for minimizing environmental footprints, pollution remediation, precision agriculture, carbon sequestration

Research Example: Treatment of Contaminated Groundwater with Iron Nanoparticles (supported by EPA and NSF)

Researchers at Lehigh University recently found that nanoscale particles of metallic iron could potentially play a large role in the remediation of contaminated groundwater (Figure 15). Interaction between iron and the pollutant trichloroethylene (TCE) results in the degradation of TCE to more environmentally benign products. Palladium or platinum is added to the nanoparticles to enhance the rate at which this reaction takes place. The researchers carried out a field demonstration at an industrial site in which nanoparticles injected into a groundwater plume containing TCE reduced contaminant levels by up to 96%. A wide variety of contaminants (including chlorinated hydrocarbons, pesticides, explosives, polychlorinated biphenyls, and perchlorate) have been successfully broken down in both laboratory and field tests. The potential for remediation stems from the high reactivity of the nanoparticles and the fact that the technology is portable and highly scalable. The high reactivity of these particles can be attributed to their extraordinarily large surface area (~33.5 m^2/g). With an average particle diameter of less than 100 nanometers, the particles are injectable and can be delivered to contaminant hot spots or source areas as needed. This work is currently being funded by EPA to explore its potential in treating hazardous waste. The technology is being tested at several Federal and industrial sites for soil and groundwater remediation.

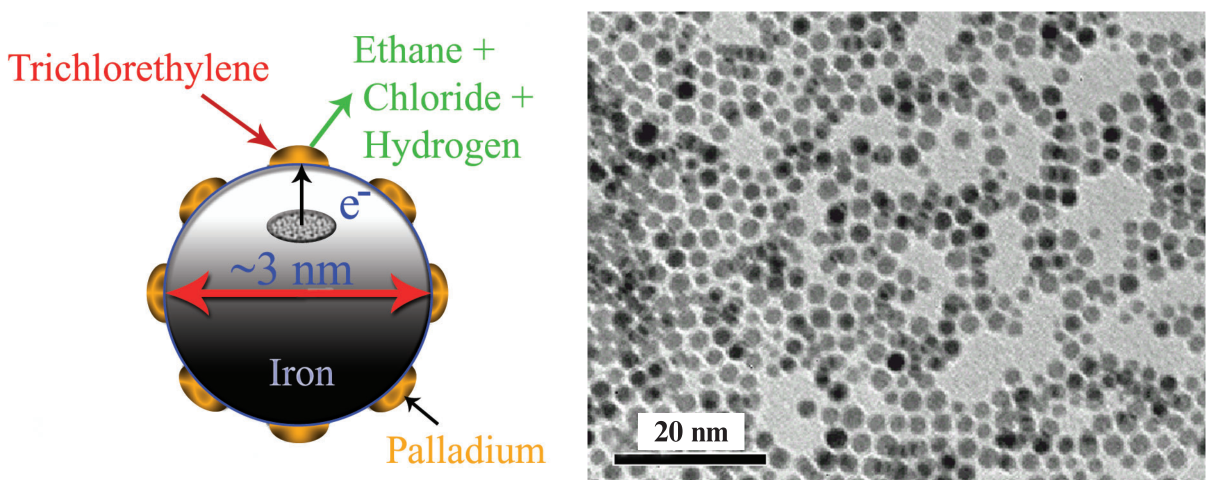


Figure 15. Schematic depiction of the remediation process in which iron nanoparticles transform a contaminant (trichloroethylene) in water into more environmentally benign products. In the process shown on the left, elemental iron acts as an electron (e-) donor while trichloroethylene serves as the electron acceptor for the chemical reaction. The presence of palladium metal on the surface of the iron nanoparticles enhances the transformation. The right portion of the figure shows a electron microscope image of the iron nanoparticles (courtesy W. Zhang, Lehigh University).